



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 AM GMT

PDB ID : 2BS4
Title : GLU C180 -> ILE VARIANT QUINOL:FUMARATE REDUCTASE FROM
WOLINELLA SUCCINOGENES
Authors : Lancaster, C.R.D.
Deposited on : 2005-05-14
Resolution : 2.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

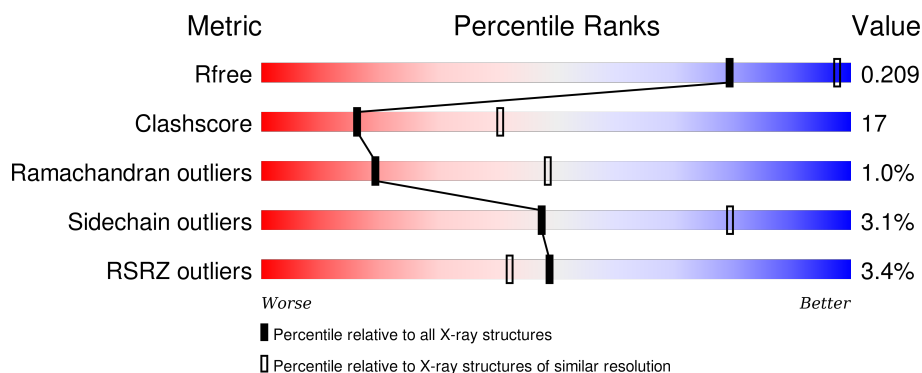
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	656	<div> <div>4%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
1	D	656	<div> <div>3%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>
2	B	239	<div> <div>%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
2	E	239	<div> <div>%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
3	C	256	<div> <div>7%</div> <div>64%</div> <div>33%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	256	<div>4% 61% 36%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	LMT	E	1242	-	-	-	X
11	LMT	F	1257	-	-	-	X
12	DMW	E	1244	-	-	-	X
12	DMW	F	1258	-	-	-	X
5	CIT	A	1657	-	-	X	X
5	CIT	D	1657	-	-	X	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 19050 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	36	0	1
			5094	3190	911	961	32			
1	D	656	Total	C	N	O	S	36	0	1
			5094	3190	911	961	32			

- Molecule 2 is a protein called QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	6	0	0
			1894	1194	322	355	23			
2	E	239	Total	C	N	O	S	6	0	0
			1894	1194	322	355	23			

- Molecule 3 is a protein called QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	255	Total	C	N	O	S	15	0	1
			2080	1389	334	343	14			
3	F	255	Total	C	N	O	S	15	0	1
			2080	1389	334	343	14			

There are 2 discrepancies between the modelled and reference sequences:

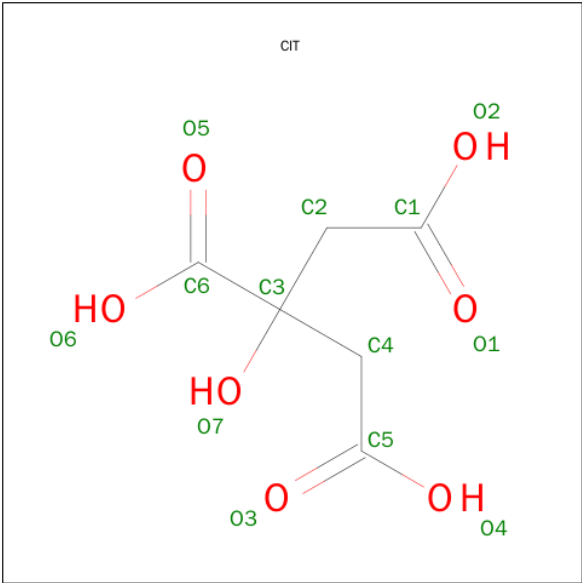
Chain	Residue	Modelled	Actual	Comment	Reference
C	180	ILE	GLU	CONFLICT SEE REMARK 9	UNP P17413
F	180	ILE	GLU	CONFLICT SEE REMARK 9	UNP P17413

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



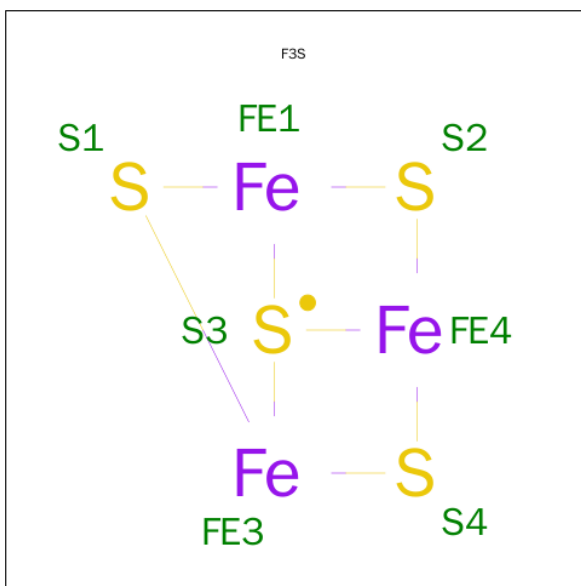
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



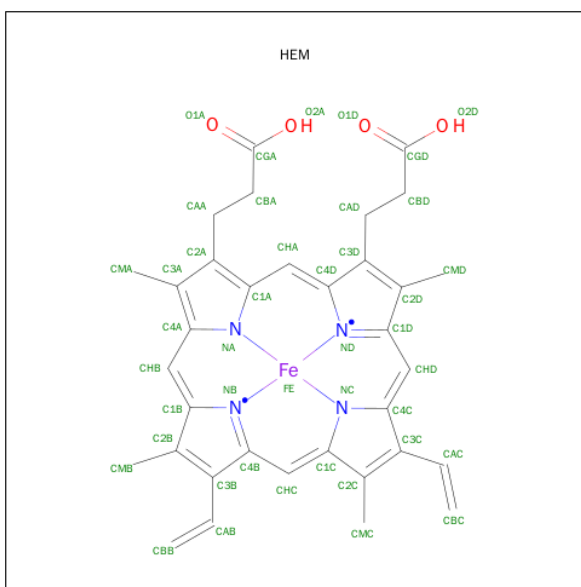
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			7	3	4		
6	E	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).

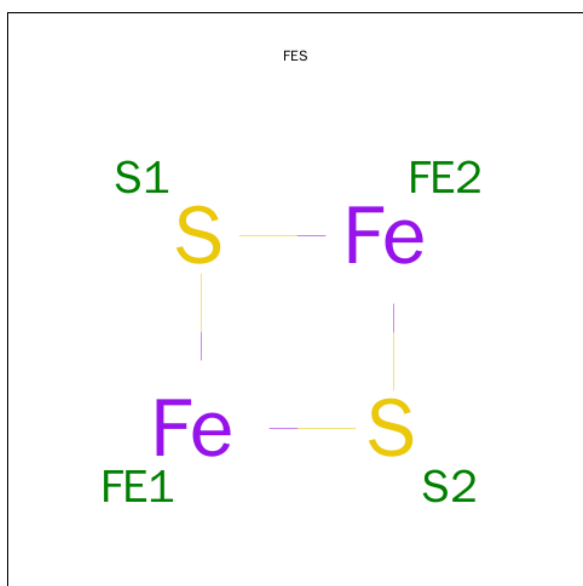


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
7	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

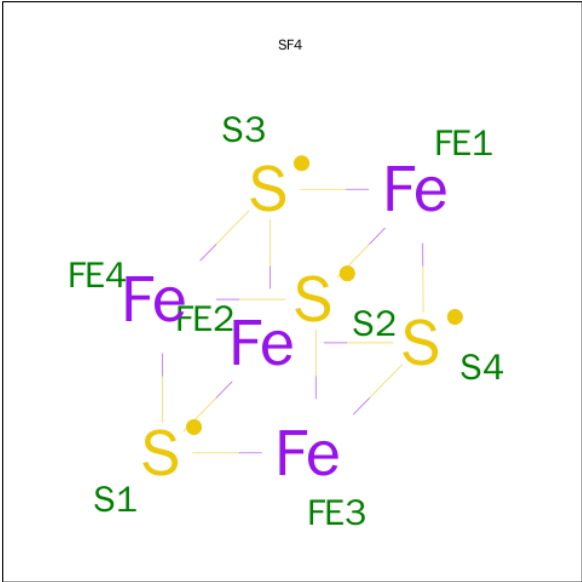
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Na		
			1	1	0	0
8	E	1	Total	Na		
			1	1	0	0

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



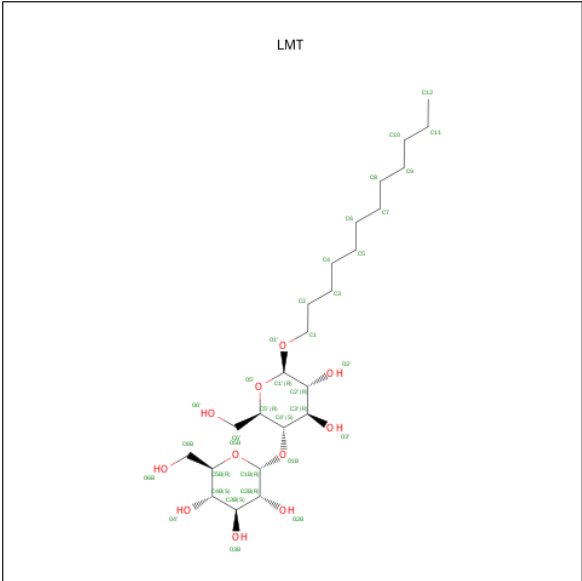
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	Fe	S		
			4	2	2	0	0
9	E	1	Total	Fe	S		
			4	2	2	0	0

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	Fe	S	0	0
			8	4	4		
10	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 11 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



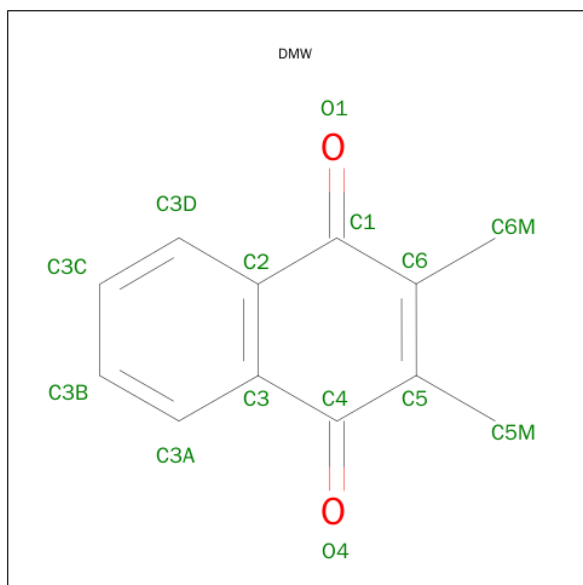
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	C	O	16	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total	C	O	16	0
			35	24	11		

- Molecule 12 is 2,3-DIMETHYL-1,4-NAPHTHOQUINONE (three-letter code: DMW) (formula: C₁₂H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	C	O	0	0
			14	12	2		
12	F	1	Total	C	O	0	0
			14	12	2		

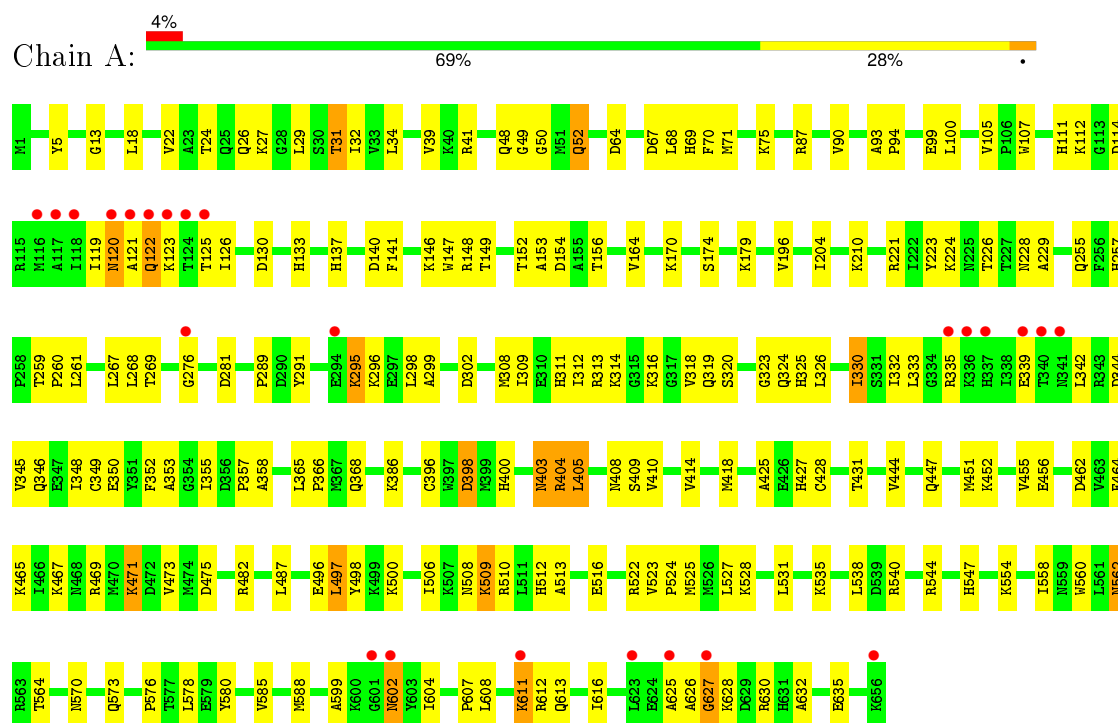
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	136	Total	O	0	0
			136	136		
13	B	73	Total	O	0	0
			73	73		
13	C	24	Total	O	0	0
			24	24		
13	D	137	Total	O	0	0
			137	137		
13	E	76	Total	O	0	0
			76	76		
13	F	26	Total	O	0	0
			26	26		

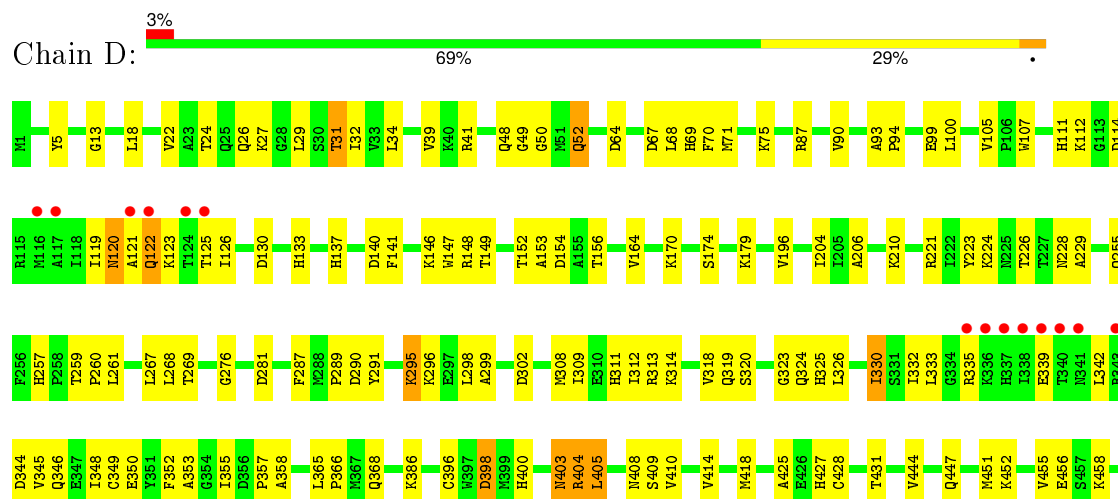
3 Residue-property plots

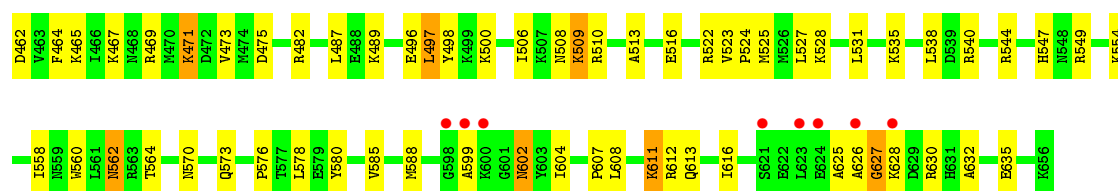
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

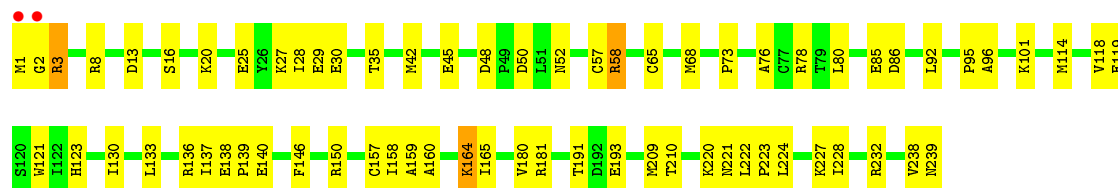


• Molecule 1: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

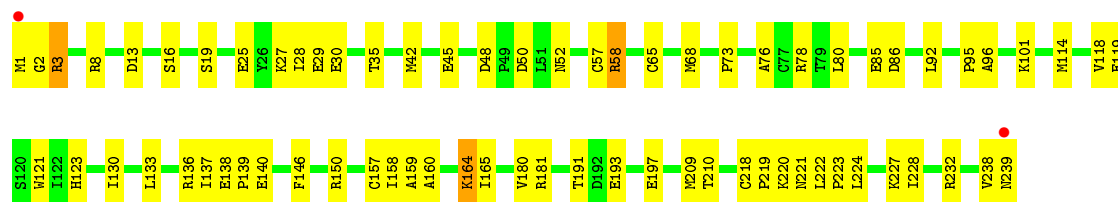




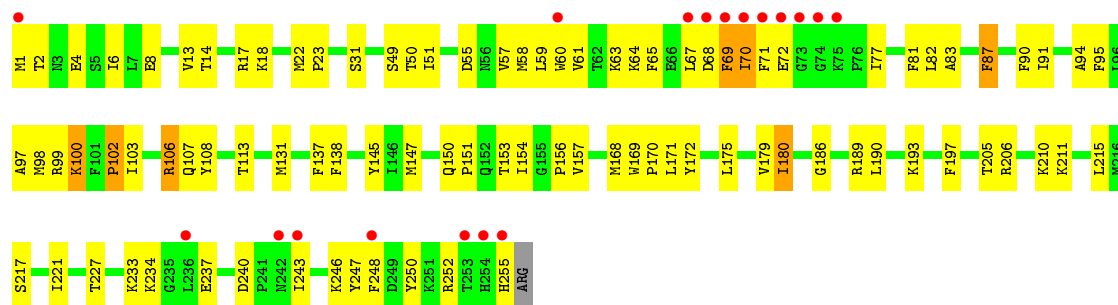
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B



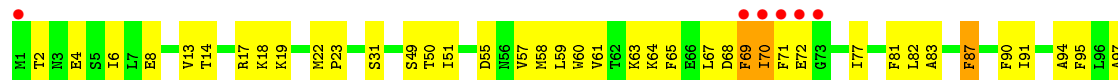
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

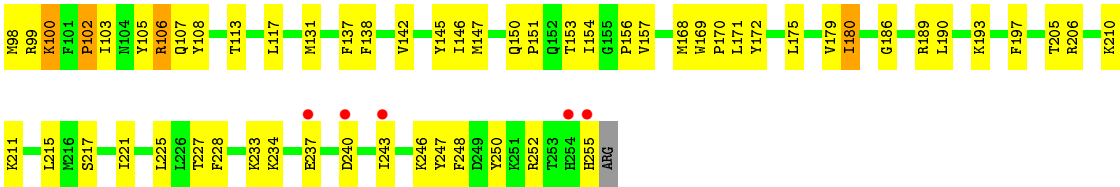


• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C



• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.10Å 188.77Å 117.82Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	29.65 – 2.76 29.71 – 2.76	Depositor EDS
% Data completeness (in resolution range)	86.0 (29.65-2.76) 85.9 (29.71-2.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.216 0.196 , 0.209	Depositor DCC
R_{free} test set	1000 reflections (1.28%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 79364 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19050	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SF4, DMW, LMT, F3S, FES, CIT, HEM, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/5190	0.62	0/6998
1	D	0.35	0/5190	0.62	0/6998
2	B	0.37	0/1931	0.62	0/2604
2	E	0.37	0/1931	0.62	0/2604
3	C	0.39	0/2146	0.55	1/2905 (0.0%)
3	F	0.39	0/2146	0.55	1/2905 (0.0%)
All	All	0.36	0/18534	0.61	2/25014 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	PRO	N-CA-C	-6.14	96.14	112.10
3	F	102	PRO	N-CA-C	-6.14	96.15	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5094	0	5069	169	0
1	D	5094	0	5069	167	0
2	B	1894	0	1861	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1894	0	1861	63	0
3	C	2080	0	2106	95	0
3	F	2080	0	2106	97	0
4	A	53	0	29	5	0
4	D	53	0	29	5	0
5	A	13	0	5	9	0
5	D	13	0	5	9	0
6	B	7	0	0	0	0
6	E	7	0	0	0	0
7	C	86	0	60	7	0
7	F	86	0	60	7	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
9	E	8	0	0	0	0
10	E	16	0	0	0	0
11	E	35	0	46	8	0
11	F	35	0	46	8	0
12	E	14	0	10	0	0
12	F	14	0	10	0	0
13	A	136	0	0	1	0
13	B	73	0	0	1	0
13	C	24	0	0	2	0
13	D	137	0	0	1	0
13	E	76	0	0	1	0
13	F	26	0	0	2	0
All	All	19050	0	18372	616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (616) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:ILE:HD12	3:F:103:ILE:CD1	1.70	1.22
3:C:103:ILE:CD1	3:F:103:ILE:HD12	1.70	1.21
1:D:112:LYS:HG3	1:D:130:ASP:HA	1.56	0.87
1:A:289:PRO:HG3	1:A:296:LYS:HG2	1.55	0.86
1:D:346:GLN:HA	1:D:357:PRO:HG3	1.56	0.86
1:D:289:PRO:HG3	1:D:296:LYS:HG2	1.55	0.86
1:A:346:GLN:HA	1:A:357:PRO:HG3	1.57	0.85
1:A:112:LYS:HG3	1:A:130:ASP:HA	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:28:ILE:HD12	2:E:42:MET:HE2	1.62	0.82
2:B:28:ILE:HD12	2:B:42:MET:HE2	1.62	0.81
3:C:98:MET:HE1	11:F:1257:LMT:H81	1.63	0.81
2:E:238:VAL:O	2:E:239:ASN:HB2	1.81	0.80
1:A:52:GLN:HG2	1:A:69:HIS:NE2	1.98	0.79
1:A:628:LYS:HG3	1:A:632:ALA:HB3	1.66	0.78
1:D:52:GLN:HG2	1:D:69:HIS:NE2	1.98	0.78
2:B:238:VAL:O	2:B:239:ASN:HB2	1.81	0.78
3:C:151:PRO:O	3:C:154:ILE:HG12	1.83	0.77
3:F:151:PRO:O	3:F:154:ILE:HG12	1.83	0.77
1:A:427:HIS:O	1:A:431:THR:HG22	1.85	0.77
1:D:628:LYS:HG3	1:D:632:ALA:HB3	1.66	0.77
1:D:427:HIS:O	1:D:431:THR:HG22	1.85	0.76
1:A:112:LYS:H	1:A:133:HIS:HD2	1.34	0.76
1:D:24:THR:OG1	1:D:31:THR:HG21	1.86	0.75
1:A:24:THR:OG1	1:A:31:THR:HG21	1.86	0.75
3:C:67:LEU:HB3	3:C:70:ILE:HD12	1.67	0.75
3:F:67:LEU:HB3	3:F:70:ILE:HD12	1.67	0.74
1:D:112:LYS:H	1:D:133:HIS:HD2	1.34	0.74
11:E:1242:LMT:H81	3:F:98:MET:HE1	1.69	0.74
1:A:267:LEU:HD23	5:A:1657:CIT:H41	1.71	0.73
1:D:179:LYS:HG3	1:D:196:VAL:HG11	1.72	0.71
1:A:261:LEU:HD13	1:A:268:LEU:HD11	1.72	0.71
1:D:267:LEU:HD23	5:D:1657:CIT:H41	1.71	0.71
1:D:261:LEU:HD13	1:D:268:LEU:HD11	1.72	0.71
1:A:179:LYS:HG3	1:A:196:VAL:HG11	1.72	0.71
3:C:4:GLU:H	3:C:4:GLU:CD	1.94	0.71
3:F:180:ILE:HD11	3:F:217:SER:HA	1.72	0.70
1:A:540:ARG:NH2	1:A:562:ASN:ND2	2.40	0.70
3:C:180:ILE:HD11	3:C:217:SER:HA	1.72	0.69
1:A:540:ARG:HH22	1:A:562:ASN:ND2	1.90	0.69
1:D:535:LYS:HG3	1:D:578:LEU:HD11	1.74	0.69
1:D:540:ARG:NH2	1:D:562:ASN:ND2	2.40	0.69
1:D:540:ARG:HH22	1:D:562:ASN:ND2	1.90	0.69
3:F:4:GLU:CD	3:F:4:GLU:H	1.94	0.69
1:A:535:LYS:HG3	1:A:578:LEU:HD11	1.74	0.68
1:A:179:LYS:HG3	1:A:196:VAL:CG1	2.24	0.67
3:F:63:LYS:HE2	3:F:68:ASP:OD2	1.95	0.67
1:D:342:LEU:O	1:D:345:VAL:HG12	1.94	0.67
3:C:63:LYS:HE2	3:C:68:ASP:OD2	1.95	0.67
1:A:342:LEU:O	1:A:345:VAL:HG12	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LYS:HG3	1:D:196:VAL:CG1	2.24	0.66
1:A:346:GLN:O	1:A:350:GLU:HG3	1.96	0.66
2:B:209:MET:SD	3:C:100:LYS:HG3	2.36	0.66
2:E:224:LEU:O	2:E:228:ILE:HG12	1.96	0.66
2:E:121:TRP:O	2:E:123:HIS:HD2	1.79	0.66
2:E:209:MET:SD	3:F:100:LYS:HG3	2.36	0.65
1:D:346:GLN:O	1:D:350:GLU:HG3	1.96	0.65
2:B:224:LEU:O	2:B:228:ILE:HG12	1.96	0.65
2:B:121:TRP:O	2:B:123:HIS:HD2	1.79	0.65
1:D:487:LEU:HB2	1:D:538:LEU:HD13	1.78	0.65
1:A:487:LEU:HB2	1:A:538:LEU:HD13	1.78	0.65
3:F:233:LYS:O	3:F:237:GLU:HG3	1.97	0.64
1:A:112:LYS:HG3	1:A:130:ASP:CA	2.28	0.64
2:E:68:MET:HB2	2:E:92:LEU:HB2	1.79	0.64
1:A:71:MET:HE3	1:A:75:LYS:HD3	1.78	0.64
1:A:612:ARG:O	1:A:616:ILE:HG12	1.98	0.64
1:D:71:MET:HE3	1:D:75:LYS:HD3	1.78	0.64
3:C:233:LYS:O	3:C:237:GLU:HG3	1.97	0.63
1:A:64:ASP:HB2	1:A:146:LYS:HG2	1.80	0.63
2:E:1:MET:SD	2:E:3:ARG:N	2.72	0.63
2:B:1:MET:SD	2:B:3:ARG:N	2.72	0.63
1:D:64:ASP:HB2	1:D:146:LYS:HG2	1.80	0.63
2:B:68:MET:HB2	2:B:92:LEU:HB2	1.79	0.62
3:F:206:ARG:O	3:F:210:LYS:HG3	1.99	0.62
1:D:612:ARG:O	1:D:616:ILE:HG12	1.98	0.62
2:E:1:MET:HA	2:E:29:GLU:CD	2.20	0.62
2:B:1:MET:HA	2:B:29:GLU:CD	2.20	0.62
2:B:146:PHE:O	2:B:150:ARG:HG3	1.98	0.62
1:A:100:LEU:HB3	1:A:105:VAL:HG21	1.81	0.62
1:A:506:ILE:HD13	1:A:508:ASN:O	1.99	0.62
1:D:112:LYS:HG3	1:D:130:ASP:CA	2.28	0.62
1:D:506:ILE:HD13	1:D:508:ASN:O	1.99	0.62
3:C:17:ARG:NH1	2:E:16:SER:O	2.33	0.62
1:D:100:LEU:HB3	1:D:105:VAL:HG21	1.81	0.62
2:E:146:PHE:O	2:E:150:ARG:HG3	1.98	0.62
3:C:60:TRP:CZ2	3:C:64:LYS:HD2	2.35	0.62
1:A:319:GLN:HE22	1:A:324:GLN:HG2	1.66	0.61
1:D:570:ASN:O	1:D:573:GLN:HG2	2.00	0.61
1:A:570:ASN:O	1:A:573:GLN:HG2	2.00	0.61
1:A:344:ASP:O	1:A:348:ILE:HG12	2.01	0.61
3:F:147:MET:HE1	3:F:154:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ILE:HG22	1:D:444:VAL:HG13	1.83	0.61
3:F:60:TRP:CZ2	3:F:64:LYS:HD2	2.35	0.61
1:D:344:ASP:O	1:D:348:ILE:HG12	2.01	0.60
3:C:206:ARG:O	3:C:210:LYS:HG3	2.00	0.60
3:C:211:LYS:O	3:C:215:LEU:HD23	2.01	0.60
1:A:255:GLN:HE21	1:A:403:ASN:ND2	1.99	0.60
1:A:204:ILE:HG22	1:A:444:VAL:HG13	1.83	0.60
1:A:257:HIS:CD2	1:A:259:THR:H	2.20	0.60
1:A:260:PRO:HD2	1:A:365:LEU:O	2.02	0.60
1:D:260:PRO:HD2	1:D:365:LEU:O	2.02	0.60
2:E:2:GLY:O	2:E:3:ARG:HG2	2.02	0.60
3:F:211:LYS:O	3:F:215:LEU:HD23	2.01	0.60
1:D:255:GLN:HE21	1:D:403:ASN:ND2	1.99	0.60
3:C:95:PHE:CE1	11:F:1257:LMT:H82	2.37	0.60
1:D:257:HIS:CD2	1:D:259:THR:H	2.19	0.60
1:A:67:ASP:OD2	1:A:630:ARG:HD2	2.02	0.60
3:F:131:MET:HG3	11:F:1257:LMT:H123	1.85	0.59
1:A:562:ASN:HD22	1:A:562:ASN:C	2.06	0.59
2:B:2:GLY:O	2:B:3:ARG:HG2	2.02	0.59
1:D:67:ASP:OD2	1:D:630:ARG:HD2	2.02	0.59
1:A:611:LYS:HZ2	1:A:611:LYS:HB3	1.67	0.59
1:D:562:ASN:C	1:D:562:ASN:HD22	2.06	0.59
1:D:611:LYS:NZ	1:D:611:LYS:HB3	2.18	0.59
2:B:16:SER:O	3:F:17:ARG:NH1	2.35	0.59
1:A:414:VAL:O	1:A:418:MET:HG3	2.02	0.59
1:D:414:VAL:O	1:D:418:MET:HG3	2.02	0.58
2:E:1:MET:HA	2:E:29:GLU:OE2	2.03	0.58
2:B:1:MET:HA	2:B:29:GLU:OE2	2.03	0.58
1:D:496:GLU:O	1:D:500:LYS:HG3	2.04	0.58
1:D:319:GLN:HE22	1:D:324:GLN:HG2	1.65	0.58
3:F:102:PRO:O	11:F:1257:LMT:H62	2.04	0.58
1:A:496:GLU:O	1:A:500:LYS:HG3	2.04	0.58
2:B:57:CYS:O	2:B:58:ARG:HG3	2.03	0.58
1:A:467:LYS:HD3	1:A:523:VAL:HG22	1.85	0.58
1:A:611:LYS:NZ	1:A:611:LYS:HB3	2.18	0.58
1:D:524:PRO:O	1:D:528:LYS:HG3	2.04	0.58
3:C:102:PRO:O	11:E:1242:LMT:H62	2.04	0.58
1:A:524:PRO:O	1:A:528:LYS:HG3	2.04	0.58
1:D:506:ILE:CG2	1:D:516:GLU:HG2	2.34	0.57
3:F:197:PHE:O	3:F:205:THR:HG21	2.05	0.57
1:D:467:LYS:HD3	1:D:523:VAL:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:119:GLU:OE1	2:E:123:HIS:HE1	1.87	0.57
2:E:57:CYS:O	2:E:58:ARG:HG3	2.03	0.57
1:D:295:LYS:HG2	1:D:299:ALA:HA	1.86	0.57
3:C:131:MET:HG3	11:E:1242:LMT:H123	1.85	0.57
1:A:632:ALA:HA	1:A:635:GLU:OE1	2.04	0.57
3:F:175:LEU:O	3:F:179:VAL:HG12	2.04	0.57
2:B:232:ARG:HD2	13:C:2019:HOH:O	2.04	0.57
2:B:13:ASP:HA	2:B:101:LYS:HG3	1.87	0.57
3:C:175:LEU:O	3:C:179:VAL:HG12	2.05	0.56
3:F:179:VAL:HG21	7:F:1256:HEM:HAC	1.87	0.56
1:D:611:LYS:HZ2	1:D:611:LYS:HB3	1.71	0.56
1:D:140:ASP:HB2	1:D:147:TRP:CE2	2.40	0.56
2:E:232:ARG:HD2	13:F:2020:HOH:O	2.05	0.56
1:A:140:ASP:HB2	1:A:147:TRP:CE2	2.40	0.56
1:D:632:ALA:HA	1:D:635:GLU:OE1	2.04	0.56
3:F:180:ILE:CD1	3:F:217:SER:HA	2.35	0.56
3:C:180:ILE:CD1	3:C:217:SER:HA	2.35	0.56
2:B:119:GLU:OE1	2:B:123:HIS:HE1	1.87	0.56
1:A:506:ILE:CG2	1:A:516:GLU:HG2	2.34	0.56
3:C:197:PHE:O	3:C:205:THR:HG21	2.05	0.56
2:E:13:ASP:HA	2:E:101:LYS:HG3	1.87	0.56
3:C:59:LEU:O	3:C:63:LYS:HG3	2.06	0.56
3:C:147:MET:HE1	3:C:154:ILE:HD12	1.88	0.56
1:A:295:LYS:HG2	1:A:299:ALA:HA	1.86	0.56
3:C:57:VAL:O	3:C:61:VAL:HG23	2.06	0.56
1:A:349:CYS:HB3	1:A:355:ILE:HG13	1.88	0.56
1:A:267:LEU:CD2	5:A:1657:CIT:H41	2.36	0.56
1:D:48:GLN:HB2	5:D:1657:CIT:O4	2.06	0.56
3:C:94:ALA:O	3:C:98:MET:HB2	2.06	0.56
1:A:464:PHE:CD1	2:B:45:GLU:HG2	2.41	0.56
3:F:57:VAL:O	3:F:61:VAL:HG23	2.06	0.56
3:F:94:ALA:O	3:F:98:MET:HB2	2.06	0.55
1:A:48:GLN:HB2	5:A:1657:CIT:O4	2.06	0.55
1:D:64:ASP:CB	1:D:146:LYS:HG2	2.36	0.55
1:D:464:PHE:CD1	2:E:45:GLU:HG2	2.41	0.55
1:D:349:CYS:HB3	1:D:355:ILE:HG13	1.88	0.55
1:D:314:LYS:NZ	1:D:314:LYS:HB3	2.21	0.55
3:F:8:GLU:HA	3:F:13:VAL:O	2.07	0.55
2:B:136:ARG:C	2:B:137:ILE:HD12	2.27	0.55
1:A:314:LYS:HB3	1:A:314:LYS:NZ	2.21	0.55
2:E:119:GLU:HG2	2:E:121:TRP:CZ2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLU:HG2	2:B:121:TRP:CZ2	2.41	0.55
2:B:164:LYS:HD3	2:B:164:LYS:O	2.06	0.55
1:A:540:ARG:HH22	1:A:562:ASN:HD22	1.55	0.55
3:F:2:THR:OG1	3:F:4:GLU:HG2	2.07	0.55
2:B:157:CYS:SG	2:B:158:ILE:HD12	2.47	0.55
3:F:171:LEU:C	3:F:171:LEU:HD23	2.28	0.55
2:E:164:LYS:HD3	2:E:164:LYS:O	2.06	0.55
3:C:179:VAL:HG21	7:C:1256:HEM:HAC	1.87	0.54
3:F:59:LEU:O	3:F:63:LYS:HG3	2.06	0.54
3:C:2:THR:OG1	3:C:4:GLU:HG2	2.07	0.54
3:F:180:ILE:HD13	3:F:180:ILE:O	2.07	0.54
1:D:319:GLN:NE2	1:D:324:GLN:HG2	2.22	0.54
1:D:22:VAL:O	1:D:26:GLN:HG2	2.08	0.54
2:E:73:PRO:HG3	2:E:160:ALA:HB2	1.90	0.54
1:A:64:ASP:CB	1:A:146:LYS:HG2	2.36	0.54
1:A:319:GLN:NE2	1:A:324:GLN:HG2	2.22	0.54
3:C:171:LEU:HD23	3:C:171:LEU:C	2.28	0.54
3:C:180:ILE:O	3:C:180:ILE:HD13	2.07	0.54
1:A:498:TYR:HA	1:A:527:LEU:HD13	1.89	0.54
3:C:186:GLY:O	3:C:190:LEU:HB2	2.08	0.54
1:D:498:TYR:HA	1:D:527:LEU:HD13	1.89	0.54
3:C:106:ARG:NH2	3:F:8:GLU:O	2.41	0.54
1:A:32:ILE:HD13	1:A:174:SER:HB3	1.90	0.54
1:D:455:VAL:O	1:D:509:LYS:HD2	2.08	0.54
1:D:267:LEU:CD2	5:D:1657:CIT:H41	2.36	0.54
2:B:158:ILE:N	2:B:158:ILE:HD12	2.23	0.54
2:E:136:ARG:C	2:E:137:ILE:HD12	2.27	0.54
3:F:55:ASP:HB3	3:F:156:PRO:HG3	1.90	0.54
1:D:540:ARG:HH22	1:D:562:ASN:HD22	1.55	0.53
1:A:469:ARG:HG3	1:A:497:LEU:HD21	1.90	0.53
1:D:18:LEU:HB3	1:D:164:VAL:HG12	1.90	0.53
3:C:8:GLU:HA	3:C:13:VAL:O	2.07	0.53
1:A:607:PRO:HG2	1:A:608:LEU:HD12	1.90	0.53
1:A:259:THR:N	1:A:260:PRO:HD3	2.24	0.53
3:F:186:GLY:O	3:F:190:LEU:HB2	2.08	0.53
3:C:6:ILE:HD13	3:F:113:THR:HG23	1.88	0.53
2:B:223:PRO:O	2:B:227:LYS:HB2	2.08	0.53
2:E:220:LYS:HB2	2:E:222:LEU:HD13	1.90	0.53
1:A:22:VAL:O	1:A:26:GLN:HG2	2.08	0.53
1:D:607:PRO:HG2	1:D:608:LEU:HD12	1.90	0.53
3:C:77:ILE:HG12	3:C:81:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:157:CYS:SG	2:E:158:ILE:HD12	2.47	0.53
1:A:455:VAL:O	1:A:509:LYS:HD2	2.08	0.53
1:D:506:ILE:O	1:D:506:ILE:HD12	2.09	0.53
3:F:77:ILE:HG12	3:F:81:PHE:HE1	1.74	0.53
1:D:469:ARG:HG3	1:D:497:LEU:HD21	1.90	0.53
11:E:1242:LMT:H82	3:F:95:PHE:CE1	2.43	0.53
2:B:73:PRO:HG3	2:B:160:ALA:HB2	1.90	0.53
1:A:309:ILE:O	1:A:313:ARG:HG3	2.09	0.53
4:D:1656:FAD:N5	5:D:1657:CIT:H22	2.24	0.53
1:A:506:ILE:O	1:A:506:ILE:HD12	2.09	0.53
1:A:554:LYS:HG2	1:A:602:ASN:ND2	2.24	0.53
1:D:554:LYS:HG2	1:D:602:ASN:ND2	2.24	0.53
1:D:309:ILE:O	1:D:313:ARG:HG3	2.09	0.53
2:B:85:GLU:HA	2:B:85:GLU:OE2	2.08	0.53
1:D:32:ILE:HD13	1:D:174:SER:HB3	1.90	0.53
2:B:220:LYS:HB2	2:B:222:LEU:HD13	1.90	0.53
1:D:259:THR:N	1:D:260:PRO:HD3	2.24	0.52
2:E:223:PRO:O	2:E:227:LYS:HB2	2.08	0.52
3:C:6:ILE:HD13	3:F:113:THR:CG2	2.40	0.52
1:A:18:LEU:HB3	1:A:164:VAL:HG12	1.90	0.52
2:E:158:ILE:HD12	2:E:158:ILE:N	2.23	0.52
2:E:85:GLU:OE2	2:E:85:GLU:HA	2.08	0.52
3:F:49:SER:HA	3:F:227:THR:CG2	2.40	0.52
4:A:1656:FAD:N5	5:A:1657:CIT:H22	2.24	0.52
1:A:141:PHE:HZ	5:A:1657:CIT:O1	1.93	0.52
3:C:49:SER:HA	3:C:227:THR:CG2	2.40	0.52
2:B:114:MET:O	2:B:118:VAL:HG22	2.11	0.52
1:A:221:ARG:HD2	1:A:226:THR:HG21	1.92	0.51
3:C:113:THR:HG23	3:F:6:ILE:HD13	1.90	0.51
1:D:522:ARG:HA	1:D:525:MET:HE3	1.93	0.51
1:A:24:THR:O	1:A:29:LEU:HB2	2.10	0.51
1:D:153:ALA:HB3	2:E:146:PHE:CZ	2.46	0.51
3:C:55:ASP:HB3	3:C:156:PRO:HG3	1.90	0.51
1:A:27:LYS:HD2	1:A:425:ALA:HB1	1.92	0.51
1:D:24:THR:O	1:D:29:LEU:HB2	2.10	0.51
2:E:65:CYS:HB2	2:E:76:ALA:HB3	1.93	0.51
3:F:131:MET:CG	11:F:1257:LMT:H123	2.40	0.51
3:C:131:MET:CG	11:E:1242:LMT:H123	2.40	0.51
3:C:145:TYR:OH	3:F:170:PRO:HG2	2.11	0.51
1:D:152:THR:OG1	1:D:156:THR:HA	2.11	0.51
1:A:120:ASN:CB	1:A:298:LEU:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:HIS:CE1	5:D:1657:CIT:O6	2.64	0.51
1:A:276:GLY:HA3	1:A:333:LEU:HD21	1.92	0.51
2:B:65:CYS:HB2	2:B:76:ALA:HB3	1.93	0.51
1:D:221:ARG:HD2	1:D:226:THR:HG21	1.92	0.51
1:A:257:HIS:CE1	5:A:1657:CIT:O6	2.64	0.51
1:D:141:PHE:HZ	5:D:1657:CIT:O1	1.93	0.51
1:D:27:LYS:HD2	1:D:425:ALA:HB1	1.92	0.51
1:A:325:HIS:HD2	1:A:326:LEU:O	1.94	0.51
1:A:152:THR:OG1	1:A:156:THR:HA	2.11	0.51
2:E:114:MET:O	2:E:118:VAL:HG22	2.11	0.50
3:F:97:ALA:HB1	7:F:1255:HEM:C2D	2.46	0.50
1:D:613:GLN:O	1:D:616:ILE:HB	2.12	0.50
1:A:153:ALA:HB3	2:B:146:PHE:CZ	2.46	0.50
1:D:319:GLN:HE22	1:D:324:GLN:CG	2.25	0.50
1:D:352:PHE:CZ	2:E:78:ARG:HG3	2.46	0.50
1:D:120:ASN:CB	1:D:298:LEU:HD11	2.41	0.50
1:D:276:GLY:HA3	1:D:333:LEU:HD21	1.92	0.50
1:A:224:LYS:HB3	1:A:475:ASP:OD2	2.11	0.50
11:E:1242:LMT:H42	3:F:95:PHE:CZ	2.47	0.50
1:D:224:LYS:HB3	1:D:475:ASP:OD2	2.11	0.50
1:D:325:HIS:HD2	1:D:326:LEU:O	1.94	0.50
1:A:613:GLN:O	1:A:616:ILE:HB	2.12	0.50
3:F:60:TRP:O	3:F:64:LYS:HG3	2.12	0.50
3:C:97:ALA:HB1	7:C:1255:HEM:C2D	2.46	0.50
3:C:60:TRP:O	3:C:64:LYS:HG3	2.12	0.50
1:A:482:ARG:HH11	1:A:547:HIS:CD2	2.30	0.49
1:A:585:VAL:HG12	1:A:612:ARG:HG2	1.94	0.49
1:A:319:GLN:HE22	1:A:324:GLN:CG	2.25	0.49
1:A:352:PHE:CZ	2:B:78:ARG:HG3	2.46	0.49
3:C:138:PHE:CE2	3:F:91:ILE:HD13	2.47	0.49
1:D:111:HIS:HA	1:D:133:HIS:CD2	2.47	0.49
3:C:95:PHE:CZ	11:F:1257:LMT:H42	2.48	0.49
4:A:1656:FAD:N5	5:A:1657:CIT:H42	2.27	0.49
3:C:99:ARG:HA	3:F:103:ILE:HG12	1.95	0.49
3:F:59:LEU:HD22	3:F:252:ARG:NH1	2.27	0.49
1:A:111:HIS:HA	1:A:133:HIS:CD2	2.47	0.49
1:D:540:ARG:NH2	1:D:562:ASN:HD21	2.10	0.49
1:D:342:LEU:HB3	1:D:345:VAL:CG1	2.43	0.49
1:D:112:LYS:H	1:D:133:HIS:CD2	2.24	0.49
1:D:482:ARG:HH11	1:D:547:HIS:CD2	2.30	0.49
2:B:48:ASP:OD1	2:B:50:ASP:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:87:PHE:O	3:F:91:ILE:HG12	2.13	0.49
1:D:308:MET:O	1:D:312:ILE:HG13	2.13	0.49
3:F:147:MET:HE2	7:F:1256:HEM:HHB	1.94	0.49
3:C:69:PHE:C	3:C:70:ILE:HG13	2.33	0.49
3:C:91:ILE:HD13	3:F:138:PHE:CE2	2.47	0.49
3:C:147:MET:CE	3:C:154:ILE:HD12	2.42	0.49
1:A:5:TYR:C	1:A:5:TYR:CD1	2.86	0.49
3:F:147:MET:CE	3:F:154:ILE:HD12	2.42	0.49
1:A:64:ASP:HB2	1:A:146:LYS:CG	2.42	0.49
1:D:64:ASP:HB2	1:D:146:LYS:CG	2.42	0.49
3:F:168:MET:C	3:F:170:PRO:HD2	2.33	0.49
1:A:308:MET:O	1:A:312:ILE:HG13	2.13	0.49
4:D:1656:FAD:N5	5:D:1657:CIT:H42	2.27	0.48
1:A:540:ARG:NH2	1:A:562:ASN:HD21	2.10	0.48
1:A:342:LEU:HB3	1:A:345:VAL:CG1	2.43	0.48
3:C:168:MET:C	3:C:170:PRO:HD2	2.33	0.48
1:D:5:TYR:CD1	1:D:5:TYR:C	2.86	0.48
3:F:50:THR:HG21	3:F:61:VAL:HG21	1.95	0.48
3:C:170:PRO:HG2	3:F:145:TYR:OH	2.13	0.48
3:F:14:THR:HG23	3:F:18:LYS:O	2.13	0.48
1:D:585:VAL:HG12	1:D:612:ARG:HG2	1.94	0.48
3:C:14:THR:HG23	3:C:18:LYS:O	2.13	0.48
2:E:95:PRO:HD2	2:E:159:ALA:HB1	1.95	0.48
3:C:59:LEU:HD22	3:C:252:ARG:NH1	2.27	0.48
1:A:513:ALA:HB1	2:B:52:ASN:HD21	1.78	0.48
3:C:87:PHE:O	3:C:91:ILE:HG12	2.13	0.48
1:A:335:ARG:NH1	1:A:358:ALA:HB3	2.29	0.48
1:A:342:LEU:HD12	1:A:342:LEU:N	2.28	0.48
2:E:8:ARG:HG2	2:E:25:GLU:HG2	1.95	0.48
3:F:69:PHE:C	3:F:70:ILE:HG13	2.33	0.48
4:A:1656:FAD:H9	13:A:2081:HOH:O	2.14	0.48
1:A:365:LEU:HD12	1:A:366:PRO:HD2	1.95	0.48
1:D:342:LEU:HD12	1:D:342:LEU:N	2.28	0.48
1:A:452:LYS:O	1:A:456:GLU:HG3	2.14	0.48
1:A:604:ILE:N	1:A:604:ILE:HD12	2.29	0.48
3:C:65:PHE:C	3:C:67:LEU:H	2.16	0.48
3:C:50:THR:HG21	3:C:61:VAL:HG21	1.95	0.48
1:A:120:ASN:HB3	1:A:298:LEU:HD11	1.95	0.48
2:E:48:ASP:OD1	2:E:50:ASP:HB3	2.13	0.48
2:B:8:ARG:HG2	2:B:25:GLU:HG2	1.95	0.48
1:D:558:ILE:HD12	1:D:604:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:ILE:HG23	2:E:164:LYS:HG2	1.96	0.48
3:C:6:ILE:HD12	3:F:117:LEU:HD11	1.95	0.48
2:B:27:LYS:HA	2:B:27:LYS:HE2	1.96	0.48
3:F:65:PHE:C	3:F:67:LEU:H	2.16	0.47
2:B:158:ILE:HG23	2:B:164:LYS:HG2	1.96	0.47
3:F:169:TRP:N	3:F:170:PRO:HD2	2.29	0.47
1:D:120:ASN:HB3	1:D:298:LEU:HD11	1.95	0.47
1:D:452:LYS:O	1:D:456:GLU:HG3	2.14	0.47
1:A:558:ILE:HD12	1:A:604:ILE:CG2	2.43	0.47
1:D:604:ILE:N	1:D:604:ILE:HD12	2.28	0.47
3:C:147:MET:HE2	7:C:1256:HEM:HHB	1.96	0.47
4:D:1656:FAD:H9	13:D:2082:HOH:O	2.13	0.47
2:E:121:TRP:O	2:E:123:HIS:CD2	2.64	0.47
3:C:87:PHE:O	3:C:90:PHE:HB3	2.14	0.47
3:C:69:PHE:CD1	3:C:70:ILE:HG13	2.49	0.47
1:D:365:LEU:HD12	1:D:366:PRO:HD2	1.95	0.47
1:A:314:LYS:NZ	1:A:314:LYS:CB	2.78	0.47
3:C:113:THR:CG2	3:F:6:ILE:HD13	2.44	0.47
2:E:27:LYS:HE2	2:E:27:LYS:HA	1.96	0.47
1:D:513:ALA:HB1	2:E:52:ASN:HD21	1.78	0.47
3:C:169:TRP:N	3:C:170:PRO:HD2	2.29	0.47
1:A:320:SER:HB3	1:A:323:GLY:O	2.15	0.47
3:C:63:LYS:O	3:C:68:ASP:HB2	2.15	0.47
1:A:319:GLN:HE22	1:A:324:GLN:CD	2.18	0.47
3:F:87:PHE:O	3:F:90:PHE:HB3	2.14	0.47
1:D:335:ARG:NH1	1:D:358:ALA:HB3	2.29	0.47
1:A:70:PHE:HA	1:A:90:VAL:HG11	1.97	0.47
2:E:210:THR:HG22	2:E:210:THR:O	2.15	0.47
2:E:210:THR:O	3:F:189:ARG:NH1	2.48	0.47
2:B:95:PRO:HD2	2:B:159:ALA:HB1	1.95	0.47
1:D:320:SER:HB3	1:D:323:GLY:O	2.15	0.47
1:D:540:ARG:NH2	1:D:562:ASN:HD22	2.11	0.47
3:F:63:LYS:O	3:F:68:ASP:HB2	2.15	0.47
1:D:608:LEU:HD12	1:D:608:LEU:H	1.80	0.47
1:D:119:ILE:HB	1:D:122:GLN:O	2.15	0.47
2:B:210:THR:O	2:B:210:THR:HG22	2.15	0.47
1:D:70:PHE:HA	1:D:90:VAL:HG11	1.97	0.47
1:D:170:LYS:HG3	2:E:121:TRP:CE2	2.50	0.46
1:A:608:LEU:HD12	1:A:608:LEU:H	1.80	0.46
1:A:462:ASP:HB3	1:A:465:LYS:HD3	1.97	0.46
1:A:52:GLN:HB3	1:A:408:ASN:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:SER:O	3:C:221:ILE:HG13	2.16	0.46
2:E:2:GLY:O	2:E:3:ARG:CB	2.63	0.46
3:F:60:TRP:CE2	3:F:64:LYS:HD2	2.50	0.46
1:D:319:GLN:HE22	1:D:324:GLN:CD	2.18	0.46
1:A:314:LYS:HZ3	1:A:314:LYS:HB3	1.80	0.46
1:D:107:TRP:HA	1:D:152:THR:HG22	1.97	0.46
3:F:69:PHE:CD1	3:F:70:ILE:HG13	2.49	0.46
3:C:108:TYR:CD1	11:E:1242:LMT:H2'	2.51	0.46
1:A:170:LYS:HG3	2:B:121:TRP:CE2	2.50	0.46
3:C:60:TRP:CE2	3:C:64:LYS:HD2	2.50	0.46
1:D:608:LEU:N	1:D:608:LEU:HD12	2.30	0.46
1:A:228:ASN:HD22	1:A:228:ASN:N	2.12	0.46
3:F:108:TYR:CD1	11:F:1257:LMT:H2'	2.51	0.46
2:B:121:TRP:O	2:B:123:HIS:CD2	2.64	0.46
1:A:469:ARG:O	1:A:473:VAL:HG23	2.15	0.46
3:C:77:ILE:HG12	3:C:81:PHE:CE1	2.50	0.46
1:A:107:TRP:HA	1:A:152:THR:HG22	1.97	0.46
1:D:604:ILE:H	1:D:604:ILE:HD12	1.81	0.46
1:D:228:ASN:N	1:D:228:ASN:HD22	2.12	0.46
3:F:217:SER:O	3:F:221:ILE:HG13	2.16	0.46
1:D:554:LYS:HG2	1:D:602:ASN:HD22	1.80	0.46
1:A:119:ILE:HB	1:A:122:GLN:O	2.15	0.46
1:A:604:ILE:H	1:A:604:ILE:HD12	1.81	0.46
1:D:64:ASP:HA	1:D:68:LEU:HD12	1.97	0.46
1:A:608:LEU:HD12	1:A:608:LEU:N	2.30	0.46
1:A:554:LYS:HG2	1:A:602:ASN:HD22	1.80	0.46
2:B:210:THR:O	3:C:189:ARG:NH1	2.48	0.46
3:C:103:ILE:H	3:C:107:GLN:NE2	2.14	0.46
3:F:147:MET:HE2	7:F:1256:HEM:CHB	2.46	0.46
1:A:64:ASP:HA	1:A:68:LEU:HD12	1.97	0.46
1:D:462:ASP:HB3	1:D:465:LYS:HD3	1.97	0.46
3:F:103:ILE:H	3:F:107:GLN:NE2	2.14	0.46
1:D:314:LYS:CB	1:D:314:LYS:NZ	2.78	0.46
2:B:96:ALA:HB2	2:B:165:ILE:HD13	1.97	0.46
1:D:52:GLN:HB3	1:D:408:ASN:HD22	1.81	0.46
2:E:96:ALA:HB2	2:E:165:ILE:HD13	1.97	0.46
1:A:410:VAL:HG22	4:A:1656:FAD:O2	2.15	0.45
1:D:410:VAL:HG22	4:D:1656:FAD:O2	2.15	0.45
2:B:2:GLY:O	2:B:3:ARG:CB	2.63	0.45
1:A:625:ALA:C	1:A:627:GLY:H	2.19	0.45
3:C:246:LYS:HG2	3:C:247:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ALA:HB3	1:D:94:PRO:HD3	1.98	0.45
1:A:396:CYS:C	1:A:398:ASP:N	2.67	0.45
1:A:123:LYS:H	1:A:123:LYS:HG2	1.58	0.45
3:F:246:LYS:HG2	3:F:247:TYR:CE1	2.51	0.45
3:C:150:GLN:N	3:C:151:PRO:CD	2.79	0.45
1:D:469:ARG:O	1:D:473:VAL:HG23	2.15	0.45
1:D:625:ALA:C	1:D:627:GLY:H	2.19	0.45
1:A:52:GLN:HB2	1:A:52:GLN:HE21	1.46	0.45
3:F:168:MET:HB3	3:F:172:TYR:CE2	2.51	0.45
3:F:77:ILE:HG12	3:F:81:PHE:CE1	2.50	0.45
3:C:168:MET:HB3	3:C:172:TYR:CE2	2.51	0.45
3:F:153:THR:HG21	3:F:246:LYS:HD2	1.99	0.45
1:D:346:GLN:HA	1:D:357:PRO:CG	2.39	0.45
1:A:560:TRP:HZ3	1:A:580:TYR:CE2	2.35	0.45
3:C:103:ILE:HG12	3:F:99:ARG:HA	1.97	0.45
1:D:261:LEU:HD21	1:D:353:ALA:HB2	1.98	0.45
3:C:17:ARG:HD2	2:E:19:SER:O	2.16	0.45
3:C:153:THR:HG21	3:C:246:LYS:HD2	1.99	0.45
1:D:112:LYS:CD	1:D:130:ASP:HB3	2.47	0.45
1:A:52:GLN:HG3	1:A:148:ARG:HD2	1.99	0.45
2:E:52:ASN:CG	2:E:101:LYS:HE3	2.37	0.45
1:A:13:GLY:HA3	1:A:39:VAL:HG12	1.99	0.45
1:D:49:GLY:HA3	5:D:1657:CIT:O7	2.17	0.45
1:D:560:TRP:HZ3	1:D:580:TYR:CE2	2.35	0.45
4:D:1656:FAD:H9	4:D:1656:FAD:H1'1	1.71	0.44
1:A:540:ARG:NH2	1:A:562:ASN:HD22	2.11	0.44
1:A:221:ARG:HD3	1:A:229:ALA:O	2.18	0.44
1:A:93:ALA:HB3	1:A:94:PRO:HD3	1.98	0.44
2:B:138:GLU:HB3	2:B:140:GLU:OE1	2.17	0.44
3:F:150:GLN:N	3:F:151:PRO:CD	2.79	0.44
1:D:29:LEU:O	1:D:31:THR:HG23	2.17	0.44
1:A:261:LEU:HD21	1:A:353:ALA:HB2	1.98	0.44
1:A:531:LEU:O	1:A:535:LYS:HB3	2.17	0.44
2:B:52:ASN:CG	2:B:101:LYS:HE3	2.37	0.44
1:D:396:CYS:C	1:D:398:ASP:N	2.67	0.44
2:E:138:GLU:HB3	2:E:140:GLU:OE1	2.17	0.44
3:C:102:PRO:O	11:E:1242:LMT:C6	2.66	0.44
1:A:261:LEU:CD1	1:A:268:LEU:HD11	2.44	0.44
1:A:29:LEU:O	1:A:31:THR:HG23	2.17	0.44
3:C:168:MET:HB3	3:C:172:TYR:CD2	2.53	0.44
1:A:123:LYS:HE2	1:A:123:LYS:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ARG:HA	1:A:525:MET:HE3	2.00	0.44
1:D:119:ILE:C	1:D:121:ALA:H	2.21	0.44
1:D:531:LEU:O	1:D:535:LYS:HB3	2.17	0.44
2:E:3:ARG:HE	2:E:30:GLU:CD	2.21	0.44
2:E:221:ASN:HA	13:E:2073:HOH:O	2.17	0.44
1:A:34:LEU:HD13	1:A:196:VAL:HG21	2.00	0.44
2:B:3:ARG:HE	2:B:30:GLU:CD	2.21	0.44
1:D:221:ARG:HD3	1:D:229:ALA:O	2.18	0.44
3:F:168:MET:HB3	3:F:172:TYR:CD2	2.53	0.43
3:C:190:LEU:HD13	7:C:1255:HEM:CGA	2.48	0.43
3:F:190:LEU:HD13	7:F:1255:HEM:CGA	2.48	0.43
1:D:281:ASP:HB3	1:D:311:HIS:CD2	2.54	0.43
1:A:112:LYS:CD	1:A:130:ASP:HB3	2.47	0.43
3:C:147:MET:HE2	7:C:1256:HEM:CHB	2.48	0.43
1:A:119:ILE:C	1:A:121:ALA:H	2.21	0.43
1:D:52:GLN:HG3	1:D:148:ARG:HD2	1.99	0.43
1:A:179:LYS:CG	1:A:196:VAL:HG11	2.45	0.43
1:D:487:LEU:CB	1:D:538:LEU:HD13	2.46	0.43
1:A:71:MET:HE3	1:A:75:LYS:CD	2.47	0.43
1:D:64:ASP:CG	1:D:146:LYS:HG2	2.39	0.43
1:A:141:PHE:CZ	5:A:1657:CIT:O1	2.71	0.43
4:A:1656:FAD:H1'1	4:A:1656:FAD:H9	1.71	0.43
1:A:49:GLY:HA3	5:A:1657:CIT:O7	2.17	0.43
1:D:34:LEU:HD13	1:D:196:VAL:HG21	2.00	0.43
2:E:146:PHE:CE2	2:E:150:ARG:HD2	2.54	0.43
3:C:145:TYR:CZ	3:F:171:LEU:HB2	2.53	0.43
2:E:191:THR:OG1	2:E:193:GLU:HG2	2.18	0.43
1:A:114:ASP:HA	1:A:126:ILE:O	2.19	0.43
1:D:123:LYS:HG2	1:D:123:LYS:H	1.58	0.43
1:D:114:ASP:HA	1:D:126:ILE:O	2.19	0.43
1:A:50:GLY:HA3	1:A:149:THR:CG2	2.48	0.43
2:B:191:THR:OG1	2:B:193:GLU:HG2	2.18	0.43
1:D:13:GLY:HA3	1:D:39:VAL:HG12	1.99	0.43
2:B:146:PHE:CE2	2:B:150:ARG:HD2	2.54	0.43
2:B:96:ALA:HB1	2:B:164:LYS:HD2	2.01	0.43
3:C:22:MET:HB2	3:C:23:PRO:HD3	2.01	0.43
3:C:22:MET:HG3	3:F:105:TYR:CE1	2.54	0.43
3:F:102:PRO:O	11:F:1257:LMT:C6	2.66	0.43
2:B:221:ASN:HA	13:B:2071:HOH:O	2.17	0.43
1:A:318:VAL:O	1:A:324:GLN:HA	2.19	0.43
2:E:96:ALA:HB1	2:E:164:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD13	1:A:330:ILE:H	1.84	0.43
1:A:332:ILE:C	1:A:332:ILE:HD12	2.39	0.43
1:A:223:TYR:CD1	1:A:368:GLN:HG3	2.54	0.43
1:A:540:ARG:HB3	1:A:547:HIS:CE1	2.54	0.42
1:D:71:MET:HE3	1:D:75:LYS:CD	2.47	0.42
1:D:318:VAL:O	1:D:324:GLN:HA	2.19	0.42
2:E:232:ARG:CZ	3:F:193:LYS:HD2	2.49	0.42
1:D:458:LYS:HB2	1:D:458:LYS:HE2	1.88	0.42
1:A:405:LEU:O	1:A:408:ASN:HB2	2.19	0.42
3:C:70:ILE:HB	3:C:71:PHE:CD1	2.54	0.42
1:D:141:PHE:CZ	5:D:1657:CIT:O1	2.71	0.42
1:D:540:ARG:HB3	1:D:547:HIS:CE1	2.54	0.42
1:D:540:ARG:NH1	1:D:564:THR:OG1	2.52	0.42
1:A:510:ARG:NH2	2:B:101:LYS:NZ	2.68	0.42
3:F:49:SER:HA	3:F:227:THR:HG23	2.02	0.42
1:A:281:ASP:HB3	1:A:311:HIS:CD2	2.54	0.42
2:E:28:ILE:HG23	2:E:42:MET:CE	2.49	0.42
1:D:261:LEU:CD1	1:D:268:LEU:HD11	2.45	0.42
1:D:447:GLN:O	1:D:451:MET:HG2	2.20	0.42
1:D:535:LYS:HG2	1:D:576:PRO:HG2	2.02	0.42
1:A:64:ASP:CG	1:A:146:LYS:HG2	2.39	0.42
1:A:467:LYS:O	1:A:471:LYS:HG2	2.19	0.42
2:E:180:VAL:HG11	2:E:227:LYS:HD2	2.01	0.42
1:D:50:GLY:HA3	1:D:149:THR:CG2	2.48	0.42
1:D:467:LYS:O	1:D:471:LYS:HG2	2.19	0.42
1:D:223:TYR:CD1	1:D:368:GLN:HG3	2.54	0.42
2:B:28:ILE:HG23	2:B:42:MET:CE	2.49	0.42
1:D:510:ARG:NH2	2:E:101:LYS:NZ	2.68	0.42
3:C:1:MET:SD	3:F:117:LEU:HG	2.59	0.42
1:D:332:ILE:C	1:D:332:ILE:HD12	2.39	0.42
3:F:157:VAL:HG21	3:F:248:PHE:HD2	1.85	0.42
1:D:405:LEU:O	1:D:408:ASN:HB2	2.19	0.42
1:A:27:LYS:HB3	1:A:27:LYS:HE3	1.87	0.42
1:A:112:LYS:H	1:A:133:HIS:CD2	2.24	0.42
1:A:111:HIS:HB3	2:B:139:PRO:HG3	2.02	0.42
2:E:1:MET:HG2	2:E:3:ARG:H	1.85	0.42
3:C:206:ARG:HD3	13:C:2021:HOH:O	2.20	0.42
3:F:206:ARG:HD3	13:F:2022:HOH:O	2.20	0.41
1:D:330:ILE:HD13	1:D:330:ILE:H	1.84	0.41
3:F:250:TYR:CE1	3:F:255:HIS:N	2.88	0.41
3:C:108:TYR:CD1	3:C:108:TYR:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ARG:NH1	1:A:564:THR:OG1	2.52	0.41
1:A:535:LYS:HG2	1:A:576:PRO:HG2	2.02	0.41
1:D:400:HIS:CG	1:D:404:ARG:HB2	2.56	0.41
2:B:20:LYS:HE2	2:B:20:LYS:HB3	1.92	0.41
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.85	0.41
3:C:51:ILE:HD11	3:C:234:LYS:HD3	2.02	0.41
2:B:232:ARG:CZ	3:C:193:LYS:HD2	2.49	0.41
3:C:8:GLU:O	3:F:106:ARG:NH2	2.47	0.41
1:D:111:HIS:HB3	2:E:139:PRO:HG3	2.02	0.41
3:F:70:ILE:HB	3:F:71:PHE:CD1	2.54	0.41
1:D:289:PRO:CG	1:D:296:LYS:HG2	2.39	0.41
3:C:154:ILE:N	3:C:154:ILE:HD13	2.36	0.41
1:A:400:HIS:CG	1:A:404:ARG:HB2	2.56	0.41
1:A:210:LYS:HE2	1:A:428:CYS:O	2.21	0.41
1:A:447:GLN:O	1:A:451:MET:HG2	2.20	0.41
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.85	0.41
1:D:154:ASP:OD2	1:D:344:ASP:HB2	2.21	0.41
1:A:335:ARG:O	1:A:339:GLU:HG3	2.21	0.41
3:C:157:VAL:HG21	3:C:248:PHE:HD2	1.85	0.41
2:E:218:CYS:HA	2:E:219:PRO:HD2	1.97	0.41
3:F:22:MET:HB2	3:F:23:PRO:HD3	2.01	0.41
1:A:512:HIS:O	1:A:513:ALA:C	2.59	0.41
3:F:31:SER:HA	7:F:1255:HEM:O2A	2.20	0.41
1:D:489:LYS:HE2	1:D:489:LYS:HB3	1.83	0.41
2:E:52:ASN:OD1	2:E:101:LYS:HE3	2.21	0.41
2:B:95:PRO:O	2:B:96:ALA:HB3	2.21	0.41
3:F:169:TRP:HB2	3:F:228:PHE:CZ	2.56	0.41
3:C:31:SER:HA	7:C:1255:HEM:O2A	2.20	0.41
2:B:180:VAL:HG11	2:B:227:LYS:HD2	2.01	0.41
2:B:220:LYS:HE2	2:B:220:LYS:HA	2.03	0.41
1:A:281:ASP:HB2	1:A:316:LYS:O	2.21	0.41
2:E:35:THR:HG22	2:E:80:LEU:HD23	2.02	0.41
1:D:482:ARG:HH11	1:D:547:HIS:HD2	1.69	0.41
1:A:487:LEU:CB	1:A:538:LEU:HD13	2.46	0.41
1:A:585:VAL:HG22	1:A:588:MET:HE3	2.03	0.41
1:A:154:ASP:OD2	1:A:344:ASP:HB2	2.21	0.41
1:A:70:PHE:CE1	1:A:87:ARG:HG2	2.56	0.41
1:D:123:LYS:HB3	1:D:123:LYS:HE2	1.82	0.41
3:F:51:ILE:HD11	3:F:234:LYS:HD3	2.02	0.41
1:D:210:LYS:HE2	1:D:428:CYS:O	2.21	0.41
3:C:103:ILE:H	3:C:107:GLN:HE21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:TYR:C	3:F:108:TYR:CD1	2.94	0.40
3:C:83:ALA:HA	7:C:1256:HEM:HBB1	2.03	0.40
1:A:257:HIS:CD2	1:A:267:LEU:HD11	2.56	0.40
2:B:1:MET:HG2	2:B:3:ARG:H	1.85	0.40
2:B:52:ASN:OD1	2:B:101:LYS:HE3	2.21	0.40
1:D:335:ARG:O	1:D:339:GLU:HG3	2.21	0.40
1:D:549:ARG:HA	1:D:549:ARG:HD2	1.90	0.40
3:F:154:ILE:N	3:F:154:ILE:HD13	2.36	0.40
1:D:206:ALA:HB2	1:D:444:VAL:CG2	2.52	0.40
2:E:13:ASP:HB2	2:E:101:LYS:HD2	2.03	0.40
1:D:119:ILE:O	1:D:121:ALA:N	2.54	0.40
1:D:287:PHE:O	1:D:290:ASP:HB2	2.21	0.40
1:D:257:HIS:CD2	1:D:267:LEU:HD11	2.56	0.40
1:A:342:LEU:HB3	1:A:345:VAL:HG12	2.04	0.40
3:C:49:SER:HA	3:C:227:THR:HG23	2.02	0.40
1:A:119:ILE:O	1:A:121:ALA:N	2.54	0.40
3:C:240:ASP:HB3	3:C:243:ILE:HD12	2.03	0.40
3:C:250:TYR:CE1	3:C:255:HIS:N	2.88	0.40
2:B:35:THR:HG22	2:B:80:LEU:HD23	2.02	0.40
3:F:225:LEU:HA	3:F:225:LEU:HD23	1.92	0.40
3:F:83:ALA:HA	7:F:1256:HEM:HBB1	2.03	0.40
1:A:257:HIS:O	1:A:366:PRO:HA	2.21	0.40
1:A:349:CYS:O	1:A:353:ALA:HB3	2.22	0.40
1:D:585:VAL:HG22	1:D:588:MET:HE3	2.03	0.40
1:D:291:TYR:OH	1:D:314:LYS:HD3	2.22	0.40
1:A:291:TYR:OH	1:A:314:LYS:HD3	2.22	0.40
1:A:558:ILE:HD12	1:A:604:ILE:HG21	2.03	0.40
2:E:197:GLU:OE1	3:F:19:LYS:HG3	2.21	0.40
1:D:99:GLU:HB2	2:E:130:ILE:HG21	2.04	0.40
1:A:99:GLU:HB2	2:B:130:ILE:HG21	2.04	0.40
2:E:238:VAL:O	2:E:239:ASN:CB	2.61	0.40
1:D:70:PHE:CE1	1:D:87:ARG:HG2	2.56	0.40
3:F:142:VAL:O	3:F:146:ILE:HD13	2.22	0.40
3:F:240:ASP:HB3	3:F:243:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	654/656 (100%)	613 (94%)	34 (5%)	7 (1%)	17	46
1	D	654/656 (100%)	613 (94%)	34 (5%)	7 (1%)	17	46
2	B	237/239 (99%)	220 (93%)	15 (6%)	2 (1%)	24	55
2	E	237/239 (99%)	220 (93%)	15 (6%)	2 (1%)	24	55
3	C	253/256 (99%)	239 (94%)	11 (4%)	3 (1%)	16	43
3	F	253/256 (99%)	239 (94%)	11 (4%)	3 (1%)	16	43
All	All	2288/2302 (99%)	2144 (94%)	120 (5%)	24 (1%)	19	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
2	B	3	ARG
3	C	72	GLU
1	D	122	GLN
2	E	3	ARG
3	F	72	GLU
1	A	269	THR
2	B	86	ASP
1	D	269	THR
2	E	86	ASP
1	A	120	ASN
1	D	120	ASN
1	A	599	ALA
1	A	626	ALA
1	D	599	ALA
1	D	626	ALA
1	A	398	ASP
3	C	69	PHE
1	D	398	ASP
3	F	69	PHE

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Mol	Chain	Res	Type
1	A	627	GLY
1	D	627	GLY
3	C	70	ILE
3	F	70	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	532/533 (100%)	513 (96%)	19 (4%)	42	75
1	D	532/533 (100%)	513 (96%)	19 (4%)	42	75
2	B	211/211 (100%)	207 (98%)	4 (2%)	65	89
2	E	211/211 (100%)	207 (98%)	4 (2%)	65	89
3	C	221/223 (99%)	214 (97%)	7 (3%)	46	78
3	F	221/223 (99%)	214 (97%)	7 (3%)	46	78
All	All	1928/1934 (100%)	1868 (97%)	60 (3%)	47	79

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	52	GLN
1	A	125	THR
1	A	137	HIS
1	A	295	LYS
1	A	302	ASP
1	A	330	ILE
1	A	386	LYS
1	A	403	ASN
1	A	404	ARG
1	A	405	LEU
1	A	409	SER
1	A	471	LYS
1	A	497	LEU

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Mol	Chain	Res	Type
1	A	509	LYS
1	A	544	ARG
1	A	562	ASN
1	A	602	ASN
1	A	611	LYS
2	B	58	ARG
2	B	133	LEU
2	B	164	LYS
2	B	181	ARG
3	C	58	MET
3	C	82	LEU
3	C	87	PHE
3	C	100	LYS
3	C	106	ARG
3	C	137	PHE
3	C	180	ILE
1	D	31	THR
1	D	52	GLN
1	D	125	THR
1	D	137	HIS
1	D	295	LYS
1	D	302	ASP
1	D	330	ILE
1	D	386	LYS
1	D	403	ASN
1	D	404	ARG
1	D	405	LEU
1	D	409	SER
1	D	471	LYS
1	D	497	LEU
1	D	509	LYS
1	D	544	ARG
1	D	562	ASN
1	D	602	ASN
1	D	611	LYS
2	E	58	ARG
2	E	133	LEU
2	E	164	LYS
2	E	181	ARG
3	F	58	MET
3	F	82	LEU
3	F	87	PHE

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Mol	Chain	Res	Type
3	F	100	LYS
3	F	106	ARG
3	F	137	PHE
3	F	180	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	48	GLN
1	A	57	ASN
1	A	91	ASN
1	A	133	HIS
1	A	225	ASN
1	A	228	ASN
1	A	257	HIS
1	A	319	GLN
1	A	325	HIS
1	A	403	ASN
1	A	408	ASN
1	A	430	ASN
1	A	468	ASN
1	A	547	HIS
1	A	562	ASN
1	A	586	ASN
1	A	602	ASN
1	A	631	HIS
2	B	116	GLN
2	B	123	HIS
2	B	177	ASN
3	C	107	GLN
1	D	26	GLN
1	D	48	GLN
1	D	57	ASN
1	D	91	ASN
1	D	133	HIS
1	D	225	ASN
1	D	228	ASN
1	D	257	HIS
1	D	319	GLN
1	D	325	HIS
1	D	403	ASN

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Mol	Chain	Res	Type
1	D	408	ASN
1	D	430	ASN
1	D	468	ASN
1	D	547	HIS
1	D	562	ASN
1	D	586	ASN
1	D	602	ASN
1	D	631	HIS
2	E	52	ASN
2	E	116	GLN
2	E	123	HIS
3	F	107	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FAD	A	1656	1	48,58,58	1.91	11 (22%)	54,89,89	2.00	11 (20%)
5	CIT	A	1657	-	3,12,12	0.51	0	3,17,17	1.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	F3S	B	1240	2	0,9,9	0.00	-	0,15,15	0.00	-
7	HEM	C	1255	3	30,50,50	2.86	11 (36%)	24,82,82	2.02	7 (29%)
7	HEM	C	1256	3	30,50,50	2.89	10 (33%)	24,82,82	2.34	8 (33%)
4	FAD	D	1656	1	48,58,58	1.92	10 (20%)	54,89,89	2.00	11 (20%)
5	CIT	D	1657	-	3,12,12	0.51	0	3,17,17	1.61	0
9	FES	E	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
10	SF4	E	1241	2	0,12,12	0.00	-	0,24,24	0.00	-
11	LMT	E	1242	-	36,36,36	1.11	2 (5%)	47,47,47	1.22	4 (8%)
12	DMW	E	1244	-	15,15,15	2.24	5 (33%)	22,22,22	0.80	0
9	FES	E	1245	2	0,4,4	0.00	-	0,4,4	0.00	-
6	F3S	E	1246	2	0,9,9	0.00	-	0,15,15	0.00	-
10	SF4	E	1247	2	0,12,12	0.00	-	0,24,24	0.00	-
7	HEM	F	1255	3	30,50,50	2.85	11 (36%)	24,82,82	2.02	7 (29%)
7	HEM	F	1256	3	30,50,50	2.89	10 (33%)	24,82,82	2.35	8 (33%)
11	LMT	F	1257	-	36,36,36	1.11	2 (5%)	47,47,47	1.22	4 (8%)
12	DMW	F	1258	-	15,15,15	2.23	5 (33%)	22,22,22	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	1656	1	-	0/30/50/50	0/6/6/6
5	CIT	A	1657	-	-	0/6/16/16	0/0/0/0
6	F3S	B	1240	2	-	0/0/24/24	0/0/3/3
7	HEM	C	1255	3	-	0/10/54/54	0/0/8/8
7	HEM	C	1256	3	-	0/10/54/54	0/0/8/8
4	FAD	D	1656	1	-	0/30/50/50	0/6/6/6
5	CIT	D	1657	-	-	0/6/16/16	0/0/0/0
9	FES	E	1240	2	-	0/0/4/4	0/1/1/1
10	SF4	E	1241	2	-	0/0/48/48	0/6/5/5
11	LMT	E	1242	-	-	0/21/61/61	0/2/2/2
12	DMW	E	1244	-	-	0/0/20/20	0/2/2/2
9	FES	E	1245	2	-	0/0/4/4	0/1/1/1
6	F3S	E	1246	2	-	0/0/24/24	0/0/3/3
10	SF4	E	1247	2	-	0/0/48/48	0/6/5/5
7	HEM	F	1255	3	-	0/10/54/54	0/0/8/8
7	HEM	F	1256	3	-	0/10/54/54	0/0/8/8
11	LMT	F	1257	-	-	0/21/61/61	0/2/2/2
12	DMW	F	1258	-	-	0/0/20/20	0/2/2/2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1256	HEM	C3B-C4B	-7.54	1.45	1.51
7	F	1256	HEM	C3B-C4B	-7.51	1.45	1.51
7	C	1255	HEM	C3B-C4B	-6.98	1.45	1.51
7	F	1255	HEM	C3B-C4B	-6.94	1.45	1.51
7	C	1256	HEM	C2D-C3D	-6.26	1.35	1.54
7	F	1256	HEM	C2D-C3D	-6.26	1.35	1.54
7	F	1255	HEM	C2D-C3D	-6.24	1.35	1.54
7	C	1255	HEM	C2D-C3D	-6.21	1.35	1.54
7	F	1255	HEM	C3C-CAC	-5.81	1.40	1.51
7	C	1256	HEM	C3C-CAC	-5.81	1.40	1.51
7	C	1255	HEM	C3C-CAC	-5.79	1.40	1.51
7	F	1256	HEM	C3C-CAC	-5.77	1.40	1.51
7	F	1255	HEM	C3B-CAB	-5.56	1.40	1.51
7	C	1255	HEM	C3B-CAB	-5.54	1.40	1.51
7	F	1256	HEM	C3B-CAB	-5.39	1.41	1.51
7	C	1256	HEM	C3B-CAB	-5.36	1.41	1.51
7	F	1256	HEM	C3D-C4D	-5.31	1.44	1.51
7	C	1256	HEM	C3D-C4D	-5.27	1.44	1.51
7	C	1255	HEM	C3D-C4D	-5.07	1.45	1.51
7	F	1255	HEM	C3D-C4D	-5.05	1.45	1.51
4	D	1656	FAD	PA-O2A	-4.44	1.36	1.54
4	A	1656	FAD	PA-O2A	-4.44	1.36	1.54
7	F	1256	HEM	C2C-C1C	-4.33	1.44	1.52
7	C	1256	HEM	C2C-C1C	-4.33	1.44	1.52
7	C	1255	HEM	C2C-C1C	-4.05	1.44	1.52
7	F	1255	HEM	C2C-C1C	-4.04	1.44	1.52
4	A	1656	FAD	P-O2P	-3.47	1.40	1.54
4	D	1656	FAD	P-O2P	-3.47	1.40	1.54
4	D	1656	FAD	C10-N10	-3.10	1.35	1.39
4	A	1656	FAD	C10-N10	-3.06	1.35	1.39
7	C	1256	HEM	C2B-C1B	-2.10	1.45	1.51
7	C	1255	HEM	C2B-C1B	-2.09	1.45	1.51
7	F	1255	HEM	C2B-C1B	-2.09	1.45	1.51
7	F	1256	HEM	C2B-C1B	-2.09	1.45	1.51
7	F	1255	HEM	C2D-C1D	-2.05	1.45	1.51
7	C	1255	HEM	C2D-C1D	-2.03	1.45	1.51
4	A	1656	FAD	C8-C7	2.00	1.46	1.41
4	A	1656	FAD	C5X-N5	2.08	1.38	1.35
4	D	1656	FAD	C5X-N5	2.08	1.38	1.35
7	F	1255	HEM	C1C-NC	2.08	1.38	1.36
7	C	1255	HEM	C1C-NC	2.09	1.38	1.36
7	F	1256	HEM	FE-NC	2.17	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1256	HEM	FE-NC	2.17	2.04	1.95
4	A	1656	FAD	C4A-N3A	2.42	1.39	1.35
12	F	1258	DMW	C3C-C3B	2.42	1.44	1.38
4	D	1656	FAD	C4A-N3A	2.42	1.39	1.35
12	E	1244	DMW	C3C-C3B	2.45	1.44	1.38
11	E	1242	LMT	C3'-C4'	2.85	1.60	1.52
11	F	1257	LMT	C3'-C4'	2.87	1.60	1.52
7	F	1255	HEM	CBC-CAC	2.95	1.46	1.29
7	C	1255	HEM	CBC-CAC	2.95	1.46	1.29
7	C	1256	HEM	CBB-CAB	2.99	1.46	1.29
7	F	1256	HEM	CBB-CAB	2.99	1.46	1.29
4	D	1656	FAD	C4-N3	3.05	1.38	1.33
4	A	1656	FAD	C4-N3	3.06	1.38	1.33
7	F	1256	HEM	CBC-CAC	3.12	1.47	1.29
7	C	1256	HEM	CBC-CAC	3.13	1.47	1.29
12	F	1258	DMW	C3C-C3D	3.15	1.45	1.38
12	E	1244	DMW	C3C-C3D	3.17	1.45	1.38
7	F	1255	HEM	CBB-CAB	3.28	1.48	1.29
7	C	1255	HEM	CBB-CAB	3.29	1.48	1.29
11	E	1242	LMT	O5B-C1B	3.29	1.50	1.41
11	F	1257	LMT	O5B-C1B	3.30	1.50	1.41
12	F	1258	DMW	C3D-C2	3.31	1.45	1.39
12	E	1244	DMW	C6M-C6	3.32	1.57	1.50
12	F	1258	DMW	C6M-C6	3.33	1.57	1.50
12	E	1244	DMW	C3D-C2	3.35	1.45	1.39
4	A	1656	FAD	O5'-C5'	3.54	1.59	1.44
4	D	1656	FAD	O5'-C5'	3.55	1.59	1.44
4	A	1656	FAD	C4X-C10	3.55	1.47	1.41
4	D	1656	FAD	C4X-C10	3.56	1.47	1.41
12	F	1258	DMW	C3A-C3	4.25	1.47	1.39
12	E	1244	DMW	C3A-C3	4.28	1.47	1.39
4	A	1656	FAD	O4B-C1B	4.57	1.47	1.41
4	D	1656	FAD	O4B-C1B	4.58	1.47	1.41
4	A	1656	FAD	C9A-N10	4.98	1.45	1.38
4	D	1656	FAD	C9A-N10	5.01	1.45	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1656	FAD	C1'-N10-C9A	-4.75	113.52	118.86
4	D	1656	FAD	C4X-C4-N3	-4.75	117.09	123.59
4	A	1656	FAD	C4X-C4-N3	-4.74	117.11	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1656	FAD	C1'-N10-C9A	-4.71	113.57	118.86
4	D	1656	FAD	C4X-C10-N10	-4.15	118.07	120.52
4	A	1656	FAD	C4X-C10-N10	-4.14	118.08	120.52
4	D	1656	FAD	N3A-C2A-N1A	-3.74	126.03	128.89
4	A	1656	FAD	N3A-C2A-N1A	-3.71	126.05	128.89
11	F	1257	LMT	C3'-C4'-C5'	-3.34	103.28	110.84
11	E	1242	LMT	C3'-C4'-C5'	-3.34	103.29	110.84
4	D	1656	FAD	O4B-C1B-N9A	-2.97	101.88	108.10
4	A	1656	FAD	O4B-C1B-N9A	-2.96	101.89	108.10
4	A	1656	FAD	C4-C4X-C10	-2.70	118.21	119.94
4	D	1656	FAD	C4-C4X-C10	-2.68	118.23	119.94
11	F	1257	LMT	O1'-C1'-C2'	-2.41	105.00	108.04
7	F	1255	HEM	CBA-CAA-C2A	-2.40	108.22	112.53
11	E	1242	LMT	O1'-C1'-C2'	-2.39	105.02	108.04
7	C	1255	HEM	CBA-CAA-C2A	-2.39	108.24	112.53
4	A	1656	FAD	C2B-C1B-N9A	2.12	117.53	114.29
4	D	1656	FAD	C2B-C1B-N9A	2.14	117.56	114.29
11	E	1242	LMT	O1B-C4'-C3'	2.20	112.84	107.17
11	F	1257	LMT	O1B-C4'-C3'	2.20	112.84	107.17
4	A	1656	FAD	C2A-N1A-C6A	2.31	122.90	118.77
4	D	1656	FAD	C2A-N1A-C6A	2.32	122.91	118.77
7	F	1256	HEM	CMD-C2D-C3D	2.37	124.83	114.35
7	C	1256	HEM	CMD-C2D-C3D	2.37	124.84	114.35
7	C	1255	HEM	CMD-C2D-C3D	2.41	125.01	114.35
7	F	1255	HEM	CMD-C2D-C3D	2.41	125.02	114.35
4	A	1656	FAD	P-O3P-PA	2.45	139.61	132.73
4	D	1656	FAD	P-O3P-PA	2.45	139.61	132.73
7	C	1256	HEM	C3B-CAB-CBB	2.59	128.43	124.46
7	F	1256	HEM	C3B-CAB-CBB	2.60	128.45	124.46
7	C	1256	HEM	C2D-C3D-C4D	3.08	106.72	101.50
7	F	1256	HEM	C2D-C3D-C4D	3.09	106.75	101.50
7	C	1255	HEM	C2D-C3D-C4D	3.23	106.98	101.50
7	F	1255	HEM	C2D-C3D-C4D	3.25	107.00	101.50
7	F	1255	HEM	CMB-C2B-C3B	3.34	124.86	116.53
7	F	1256	HEM	CAD-C3D-C2D	3.34	122.81	113.22
7	C	1256	HEM	CAD-C3D-C2D	3.35	122.83	113.22
7	C	1255	HEM	CMB-C2B-C3B	3.35	124.89	116.53
4	D	1656	FAD	O3P-P-O5'	3.59	112.46	102.94
4	A	1656	FAD	O3P-P-O5'	3.59	112.47	102.94
7	F	1255	HEM	CMC-C2C-C3C	3.67	125.70	116.53
7	C	1255	HEM	CMC-C2C-C3C	3.68	125.71	116.53
7	F	1255	HEM	CAD-C3D-C4D	3.77	125.78	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1255	HEM	CAD-C3D-C4D	3.79	125.85	112.47
11	F	1257	LMT	C1-O1'-C1'	4.18	121.26	113.94
11	E	1242	LMT	C1-O1'-C1'	4.19	121.26	113.94
7	F	1256	HEM	CMB-C2B-C3B	4.38	127.46	116.53
7	C	1256	HEM	CMB-C2B-C3B	4.38	127.46	116.53
7	F	1256	HEM	CBA-CAA-C2A	4.47	120.54	112.53
7	C	1256	HEM	CBA-CAA-C2A	4.47	120.54	112.53
7	C	1256	HEM	CMC-C2C-C3C	4.62	128.06	116.53
7	F	1256	HEM	CMC-C2C-C3C	4.62	128.06	116.53
7	C	1255	HEM	CAD-C3D-C2D	4.86	127.18	113.22
7	F	1255	HEM	CAD-C3D-C2D	4.87	127.21	113.22
7	F	1256	HEM	CAD-C3D-C4D	5.09	130.44	112.47
7	C	1256	HEM	CAD-C3D-C4D	5.10	130.45	112.47
4	A	1656	FAD	C4-N3-C2	7.23	121.50	115.25
4	D	1656	FAD	C4-N3-C2	7.24	121.50	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1656	FAD	5	0
5	A	1657	CIT	9	0
7	C	1255	HEM	3	0
7	C	1256	HEM	4	0
4	D	1656	FAD	5	0
5	D	1657	CIT	9	0
11	E	1242	LMT	8	0
7	F	1255	HEM	3	0
7	F	1256	HEM	4	0
11	F	1257	LMT	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	656/656 (100%)	-0.34	24 (3%)	45 38	16, 34, 71, 91	15 (2%)
1	D	656/656 (100%)	-0.33	22 (3%)	49 42	16, 34, 71, 91	15 (2%)
2	B	239/239 (100%)	-0.47	2 (0%)	87 83	17, 27, 49, 88	2 (0%)
2	E	239/239 (100%)	-0.47	2 (0%)	87 83	17, 27, 49, 88	2 (0%)
3	C	255/256 (99%)	-0.05	18 (7%)	19 13	22, 44, 76, 100	10 (3%)
3	F	255/256 (99%)	-0.15	11 (4%)	39 32	22, 44, 76, 100	10 (3%)
All	All	2300/2302 (99%)	-0.31	79 (3%)	49 42	16, 34, 72, 100	54 (2%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	GLN	6.1
2	E	1	MET	6.0
2	B	1	MET	5.9
3	C	71	PHE	5.0
3	C	254	HIS	4.9
3	C	69	PHE	4.8
3	C	70	ILE	4.8
1	D	116	MET	4.7
1	A	122	GLN	4.6
3	C	72	GLU	4.2
1	D	124	THR	4.1
1	A	121	ALA	4.0
3	F	69	PHE	3.8
1	A	625	ALA	3.8
3	C	74	GLY	3.7
1	A	116	MET	3.7
1	A	124	THR	3.6
1	D	117	ALA	3.5
3	C	73	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
3	F	1	MET	3.5
3	C	67	LEU	3.4
1	D	121	ALA	3.3
1	A	337	HIS	3.3
3	F	71	PHE	3.3
3	F	240	ASP	3.3
1	D	599	ALA	3.2
3	C	68	ASP	3.2
1	A	117	ALA	3.2
1	D	624	GLU	3.2
1	D	335	ARG	3.2
1	A	339	GLU	3.1
1	D	343	ARG	3.0
1	D	125	THR	3.0
1	D	337	HIS	3.0
1	A	125	THR	3.0
1	A	601	GLY	3.0
1	A	341	ASN	3.0
1	D	336	LYS	2.9
1	D	338	ILE	2.9
3	F	243	ILE	2.9
1	D	340	THR	2.9
1	A	123	LYS	2.9
3	C	1	MET	2.8
3	C	255	HIS	2.8
3	F	70	ILE	2.8
3	C	253	THR	2.8
1	A	336	LYS	2.7
3	C	242	ASN	2.7
3	F	72	GLU	2.7
1	A	118	ILE	2.6
3	F	73	GLY	2.6
1	D	339	GLU	2.6
3	C	243	ILE	2.6
1	A	120	ASN	2.6
1	D	626	ALA	2.6
3	F	255	HIS	2.6
3	C	75	LYS	2.6
1	D	600	LYS	2.6
2	B	2	GLY	2.5
3	C	60	TRP	2.5
3	F	254	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	602	ASN	2.5
1	A	611	LYS	2.4
1	D	623	LEU	2.4
1	A	623	LEU	2.3
1	A	627	GLY	2.3
1	A	294	GLU	2.3
1	A	340	THR	2.2
1	A	656	LYS	2.2
1	A	276	GLY	2.2
1	D	621	SER	2.2
2	E	239	ASN	2.2
1	D	341	ASN	2.1
1	A	335	ARG	2.1
1	D	628	LYS	2.1
3	F	237	GLU	2.1
1	D	598	GLY	2.1
3	C	236	LEU	2.1
3	C	248	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	DMW	F	1258	14/14	0.90	0.52	19.88	27,28,29,30	14
12	DMW	E	1244	14/14	0.85	0.70	13.48	27,28,29,30	14
11	LMT	E	1242	35/35	0.76	0.42	11.53	60,65,68,68	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	LMT	F	1257	35/35	0.85	0.32	6.58	60,65,68,68	16
5	CIT	A	1657	13/13	0.79	0.40	6.23	24,28,34,35	13
5	CIT	D	1657	13/13	0.79	0.42	5.19	24,28,34,35	13
7	HEM	C	1255	43/43	0.96	0.17	0.83	29,36,39,44	0
7	HEM	F	1256	43/43	0.98	0.16	0.66	39,44,45,46	0
7	HEM	F	1255	43/43	0.97	0.14	0.44	29,36,39,44	0
7	HEM	C	1256	43/43	0.98	0.15	0.03	39,44,45,46	0
4	FAD	D	1656	53/53	0.98	0.13	-0.15	12,20,23,26	0
8	NA	D	1658	1/1	0.95	0.12	-0.18	17,17,17,17	0
4	FAD	A	1656	53/53	0.98	0.12	-0.67	12,20,23,26	0
6	F3S	B	1240	7/7	0.99	0.12	-0.95	22,23,24,26	0
8	NA	E	1243	1/1	0.93	0.10	-1.39	17,17,17,17	0
9	FES	E	1240	4/4	0.99	0.10	-1.55	19,20,21,21	0
6	F3S	E	1246	7/7	0.98	0.11	-1.61	22,23,24,26	0
9	FES	E	1245	4/4	0.99	0.09	-1.63	19,20,21,21	0
10	SF4	E	1247	8/8	0.99	0.08	-1.91	18,21,22,22	0
10	SF4	E	1241	8/8	0.99	0.07	-2.56	18,21,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.